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Random Forest Regressor based superconductivity materials investigation for critical temperature prediction

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Abstract

Ever since its invention over past hundred years, superconductivity has been the subject of intense investigation. However, numerous aspects of this unusual phenomenon stay unknown, the most notable of which being the relationship among superconductivity, compound/structural assets of materials as well. Every superconductor materials transition temperature that lies in between 1 Kelvin and 10 Kelvin. Based on critical temperature of materials, superconductivity materials classified into two namely less than 10 Kelvin, greater than 10 Kelvin. Several regression models are developed here to analyze the critical temperatures of more than 12,000 known superconductors accessible through Super Con metadata, in order to sustain. After studying and implementing the aforementioned techniques, Random Forest Regressor stood out and gave the best results in terms of R^2 score metrics initial value as 91.2% and after normalizing features in superconductivity metadata, R^2 score value reaches 92.79% in predicting the temperature values of superconductors.

Introduction

When some materials are cooled below a particular temperature, known as the superconducting critical temperature, Tc, they exhibit superconductivity. It became a focus of research after the detection of superconductors over a century in the past. The expected quantum occurrence of superconductivity is caused by the restricted magnetism among paired electrons. As mentioned in Fig. 1, two features on superconductivity materials described (a) No resistivity, and (b) ideal dia-magnetism.

There are few other characteristic properties such as resistance, impurity of materials, pressures, stress, and temperature, effects of isotopes [13], and magnetic fields that uniquely distinguish superconductors from other materials. Revathy et.al [1] proposed several regression models in predicting the critical temperature of superconducting materials with the dataset and delivered the comparisons of accuracies for each model. The work extended by performing exploratory data analysis with the dataset and by using them to predict the critical temperature. Secondly, implementing four regression models (with increased accuracy) for prediction based on certain properties like atomic mass, mean entropy, range density, thermal conductivity.

Based on these following intentions, the authors analyzed superconductivity dataset.

i. To forecast the critical temperature utilising statistical analysis of machine learning techniques, particularly regression models, based on variables derived from learning phase.

ii. Performance of novel approach shows better in foreseeing critical temperature should be possible during testing stage.

iii. Metrics such as RMSE, MSE and R^2 score value are estimated to find the performance in predicting critical temperature of superconductivity substances.

Section snippets

Background

Several authors investigated superconductivity materials using XGBoost approach [2], hybrid combination of CNN, LSTM by [3] attained R2 value of 89.9%, Bayesian Neural Network [4] achieves 92%, machine learning approach [5], regression methods [6] with 92% R2 score for predicting Tc. The authors of [7], [9] established novel superconductor materials of 3% which relied on occurrence and perception with authority proceeded in trial and error approach. The investigation done [17], [18] achieved…

Proposed Methodology

The main aim of our proposed work is to predict the T_c of the superconductors based on the features in the superconductivity dataset using machine learning [22] techniques. The basic workflow of this model is depicted in Fig. 2 illustrates that how machine based regression algorithms suitable in identifying the materials based on critical temperature.…

Metrics Evaluation

To assess if regression models are correct or deceptive, it is necessary to examine the various evaluation measures. We employ a variety of metrics such as the R^2 score, Mean Absolute Error and Mean Squared Error to assess the performance of machine learning models, particularly regression models.…

Histogram

Histograms divide data into bins and are the quickest way to see how each attribute in a dataset is distributed. The histograms used in the analysis of superconducting materials gives us a count of the number of observations of every features in each visualisation has been analyzed. The following is the histogram plot of various atomic masses comprises entropy, mean, weighted entropy, and standard atomic mass depicts in Fig. 3.…

Density plot

Density plots are also like histograms but have a smooth curve drawn …

Conclusions

In conclusion, using a basic yet robust machine learning method, specifically a regression algorithm, this study was able to predict the critical temperatures of superconducting materials using a variety of key characteristics. Several models were developed using superconductor information, with the best suited model being the Random Forest Regressor, which had R2=92.79 percent and RMSE=9.7K. Prior to the prediction, exploratory data analysis was performed to determine the association…

CRediT authorship contribution statement

G. Revathy: Conceptualization, Methodology, Software, Data curation, Writing – original draft. **V. Rajendran:** Conceptualization, Methodology, Software, Data curation, Writing – original draft. **B. Rashmika:** Visualization, Investigation. **P. Sathish Kumar:** . **P. Parkavi:** . **J. Shynisha:** Software, Validation, Writing – review & editing.…

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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